

**TURBULENT FLAME SPEED IN SPARK IGNITION ENGINE
COMBUSTION PROCESS USING COMPUTATIONAL
FLUID DYNAMICS (CFD)**

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ABSTRACT

This thesis deals with the numerical study about turbulent flame speed in spark ignition engine during the combustion process using Computational Fluid Dynamics (CFD). The objective for this project is to analyze the behavior and predicted trend of turbulent flame speed that occurs during the combustion process at single operating point for 2000 revolution per minute (rpm) engine speed. Turbulent flame speed is the important parameter that controls the cylinder pressure during combustion process in spark ignition (SI) engine. This thesis described on technique to tackle the objective starting from engine modeling until finish of the project. The analysis is focusing on spark ignition combustion process of the baseline engine design, Mitsubishi magma 4G15. Engine was modeled using Solid work software and then analysis using CFD. The engine model was design in 3-Dimensional (3D). The speed of engine is fixed at single operating point at 2000 rpm. For numerical modeling approach, k-epsilon ($k-\epsilon$) standard turbulence model was selected. The iteration number is set at 1500 iteration per time step. The accuracy test is based on cylinder pressure and the simulation data is validated with experiment data. It is known that an increase in turbulent flame speed increases the cylinder mixtures that have been burned. Thus increase the cylinder temperature and relates with the increase in cylinder pressure during the combustion process.

ABSTRAK

Tesis ini membincangkan kajian berangka tentang halaju nyalaan gelora di dalam enjin cucuhan bunga api semasa proses pembakaran menggunakan Perkomputeran Dinamik Bendalir. Tujuan utama projek ini adalah untuk menganalisa perilaku dan jangkaan corak halaju nyalaan gelora yang terjadi semasa proses pembakaran pada satu titik operasi untuk kelajuan enjin 2000 revolusi per minit (rpm). Halaju nyalaan gelora adalah parameter penting yang mengawal tekanan silinder semasa proses pembakaran dalam enjin cucuhan bunga api. Tesis ini menjelaskan tentang cara untuk mencapai tujuan bermula daripada membuat model sehingga selesai projek. Analisa memfokuskan pada proses pembakaran ke atas enjin cucuhan bunga api untuk reka bentuk enjin rujukan, Mitsubishi Magma 4G15. Enjin dimodel menggunakan perisian Solid work dan analisa menggunakan Perkomputeran Dinamik Bendalir. Model enjin telah direka bentuk dalam 3-dimensi (3D). Kelajuan enjin telah ditetapkan pada titik operasi pada 2000 rpm. Untuk pendekatan kajian berangka, k -epsilon (k - ϵ) asas model gelora telah dipilih. Bilangan lelaran ditetapkan pada 1500 sela setiap masa. Ketepatan ujian adalah berdasarkan pada tekanan silinder dan data simulasi disahkan dengan data eksperimen. Adalah diketahui bahawa peningkatan dalam halaju nyalaan gelora meningkatkan jumlah campuran silinder yang telah dibakar. Ini meningkatkan suhu silinder dan berkait dengan peningkatan dalam tekanan silinder semasa proses pembakaran.

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CHAPTER 1

INTRODUCTION

1.1 INTRODUCTION

Internal combustion engine is an engine in which the combustion takes place internally. It is combustion of a fuel occurs with an oxidizer, usually air in a combustion chamber (Pulkrabek, 1997). The combustion process in spark ignition engines plays a key role in the conversion of fuel energy into mechanical energy (Trautwein, 1990). The intake and compression stroke is one of the most important processes because it influences the pattern of air flow structure coming inside the cylinder. As the result of the high velocity inside the internal combustion engine during operation, all flow in-cylinder is typically turbulent (Kurniawan, 2007). After ignition at the spark plug, the mixture of fuel and air starts to burn and continues burning until consuming the whole of the fuel of the charge in the cylinder. The burning rate of premixed turbulent flames depends strongly on the parameters of a turbulent flow. When turbulent is sufficiently strong, then the burning rate is controlled mainly by the turbulent parameters, rather than by thermo-chemical velocity of a planar laminar flame front (Akkerman, 2009). The burning time may vary from one engine to another and each has certain burning rate. Many experiments show that the burning rate depends mostly on the combustion chamber shape and the position of the spark plug (Kodah, 1999).

The simulation of the physical process in engine combustion chamber has found increasing interest during recent years. To validate new design concept through experimental work takes a long time and high cost especially during prototype developing stage. The computer simulation techniques are useful

alternative way, provided that the simulation model is accurate and fast enough to execute. Computer simulations of internal combustion engine cycle are desirable because of the aid that they provide in design studies, in predicting trends, in serving as investigations tools, in giving more data than are normally accessible from experiments, and in helping to understand the complex process that occur inside combustion chamber (Hosseini, 2008). During the last decades, computational fluid dynamics has significantly contributed to the engine development process (Hascher, 2000). It is based on the solution of the fluid dynamic governing equations which is contains of mass, momentum, species conservation equation and energy. Additional equation for turbulence, heat transfer, spark ignition and reaction rate also required to capture all the associated combustion phenomena (Fadzil, 2008).

1.2 PROBLEM STATEMENT

It is known that combustion duration is an important parameter in spark ignition engine and mainly is controlled by turbulent flame speed. It is expected that the turbulent flame speed influence the cylinder pressure in combustion process. Thus, further analysis for turbulent flame speed in combustion process is required to identify the relation by using CFD method.

1.3 OBJECTIVE

The objective of this project is to analyze the behavior and predicted trend of turbulent flame speed at single operating point for 2000 rpm engine speed during combustion process.

1.4 SCOPES

In this study, the analysis of turbulent flame speed in spark ignition engine combustion process is carried out in the framework of turbulent flame speed closure model of Zimont using CFD. Single operating point at 2000 rpm is simulated in CFD in order to study the predicted trend and behavior of turbulent flame speed during the combustion process.

1.5 FLOW CHART

The flow chart of the overall procedure of the study is shown in Figure 1.1:

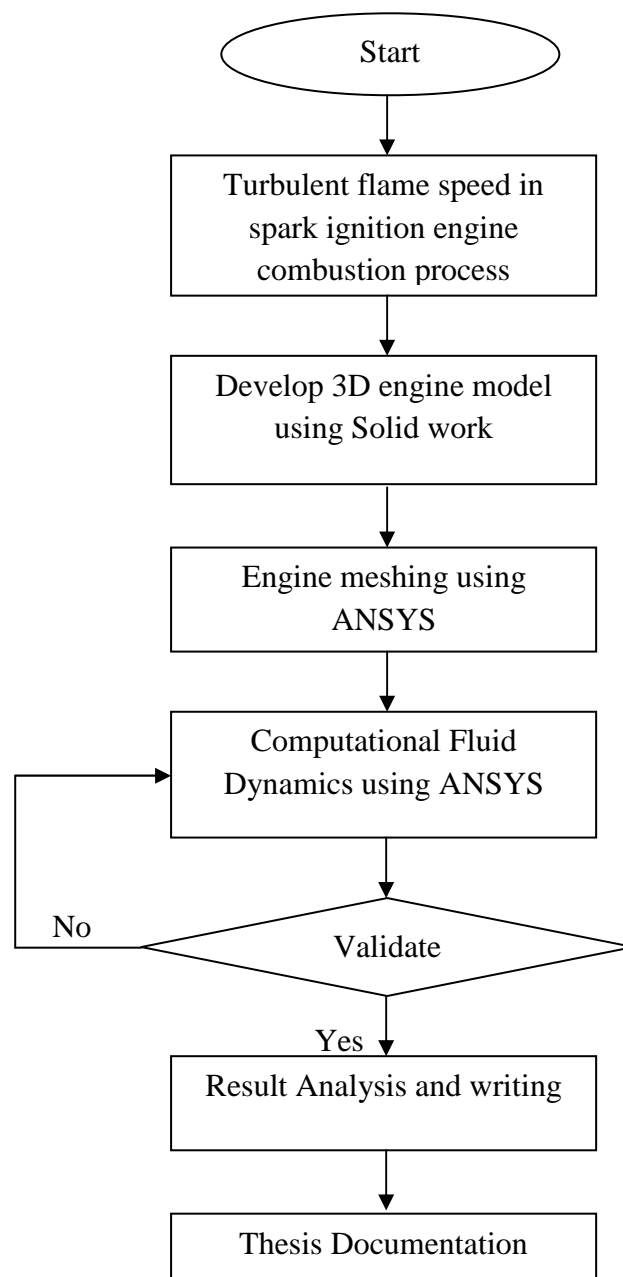


Figure 1.1: Project flow chart

1.6 ORGANIZATION OF THESIS

This thesis consists of five main chapters in order to acquire the main objective of the study related to turbulent flame speed in SI engine combustion process. The chapters are introduction, literature review, methodology, result and discussion and lastly conclusion and recommendation. Chapter 1 has briefly discussed about the introduction, problem statement, scopes of study, and also the objective of the project. Chapter 2 is literatures that related to the study and become basics of study framework. Chapter 3 presents the development of 3D model, generation of computational model and also data build in for combustion process using CFD. Chapter 4 addresses the validation of the simulated results against experimental result of the cylinder pressure and how turbulent flame speed influenced during combustion process. Chapter 5 presents the important findings of the study and recommendation for future study.

CHAPTER 2

LITERATURE REVIEW

2.1 INTRODUCTION

This chapter deals with definition of SI engine and characteristics of turbulence flow. Then this chapter continues with the importance of the study about turbulence for in-cylinder flow. Lastly, discussion continues with the characterization of flames, flame structure, laminar and turbulent flame speed.

2.2 INTERNAL COMBUSTION ENGINE

Internal combustion engine is the production of mechanical power from the chemical energy that contained in the fuel. In internal combustion engines, energy is released by burning or oxidizing the fuel inside the engine. It depends on the exothermic chemical process of combustion, which is a process or reaction that release energy usually in the form of heat, but also in the form of light (spark, flame or explosion), electricity or sound. It consists of four consecutive process which is intake, compression, expansion (including combustion) and exhaust. The work transfers which provide the desired power output occur directly between working fluids and the mechanical component of the engine (Heywood, 1998).

2.3 SPARK IGNITION ENGINE (SI ENGINE)

An SI engine starts the combustion process in each cycle by use of a spark plug. The air and fuel are usually mixed together using carburetors or fuel-injection system in the intake system prior to entry to the engine cylinder. At the combustion chamber the spark plug gives a high-voltage electrical discharge between two electrodes which ignites the air-fuel mixture that is surrounding the plug. During intake, the inducted fuel and air mix in the cylinder with the residual burned gases remaining from the previous cycle. After the intake valve close, the cylinder contents are compressed above atmospheric pressure and temperature as the cylinder volume is reduced. Between 10 and 40 crank angle degree ($^{\circ}\text{CA}$) before top dead centre (TDC) an electrical discharged across the spark plug starts the combustion process. This process is then repeated for a cycle of periods during the engine process.

Combustion duration is an important parameter in operation of spark-ignition engines and is controlled by turbulent flame speed and distribution of combustion volume. Compact combustion chambers produce short combustion durations. A turbulent flame develops from the spark discharge, propagates across the mixture of air, fuel and residual gas in the cylinder, and extinguishes at the combustion chamber wall. The duration of this burning process varies with engine design and operation.

2.4 COMBUSTION IN SI ENGINE

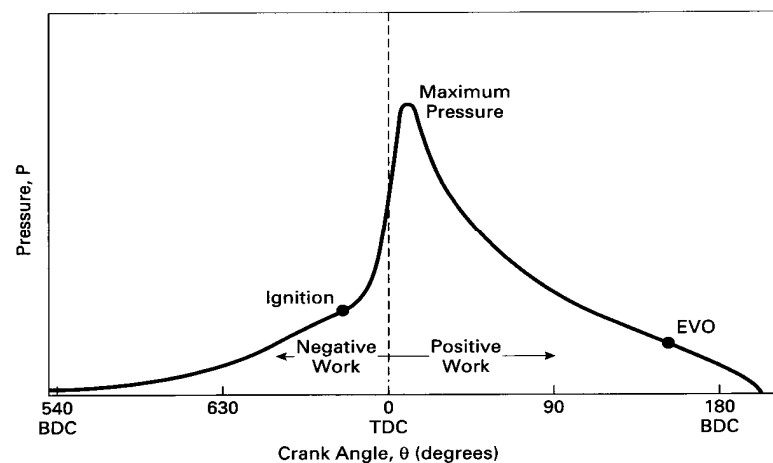
In an SI engine, combustion ideally consists of an exothermic subsonic flame progressing through a premixed homogeneous air-fuel mixture. The spread of the flame front is greatly increased by induced of turbulence, swirl and squish within the cylinder. Combustion in an engine is a very complex process. The combustion process of SI engines can be divided into three broad regions which are:

Table 2.1: Combustion process of SI engines

Stage	Combustion process
1	Ignition and flame development
2	Flame propagation
3	Flame termination

Source: (pulkrabek, 1997)

The consumption of the first 5% or 10% of the fuel air mixture is generally considered as the flame development. During this period, ignition occurs and the combustion process starts, but very little pressure rise is noticeable and little or no useful work is produced. The result of the flame propagation period of the combustion process is when just about all useful work is produced in an engine cycle. This is the period when the bulk of the fuel and air mass is burned. During this time, the pressure in the cylinder is greatly increased. And this provides the force to produced work in the expansion stroke. Flame termination is classified as the final 5% or 10% of the air-fuel mass which burns. During this time, pressure quickly decreases and the combustion stops.

**Figure 2.1:** Cylinder pressure in the combustion chamber of an SI engine

Source: (pulkrabek, 1997)

2.5 TURBULENCE FLOW

All flow into, out of, and within engine cylinders are turbulence flows due to the high velocities involved. As a result of turbulence, thermodynamics transfer rates within an engine are increased by an order of magnitude. Heat transfer, evaporation, mixing and combustion rates all increase (Pulkrabek, 1997). Certain properties could be learned about turbulence using statistical methods. These introduce certain correlation functions among flow variables. However it is impossible to determine these correlations in advance (Sodja, 2007).

In nature, almost every fluid flow is turbulent. Whenever turbulence is present in a certain flow it appears to be the dominant over all other flow phenomena. When flow is turbulent, particles experience random fluctuations in motion superimposed on their main bulk velocity. These fluctuations occur in all directions, perpendicular to the flow and in the flow direction (Pulkrabek, 1997). The characteristics of turbulence observed in nature are presented below:

Table 2.2: Turbulence model characteristics

Characteristic	Definition
Unsteadiness	Turbulence is always transient
Irregularity	The flow is so irregular that we can neither follow nor describe it completely
Three-dimensionally	Even when the mean flow is one or two-dimensional, flow fluctuations always have components in all three directions.
Dissipation	The kinetic energy of turbulent motion is dissipated into heat under the influence of viscosity
Diffusivity	The rapid mixing of momentum, heat and mass is a typical feature of turbulent flows.
Others	Turbulence occurs at higher Reynolds number and it is not a property of the particular itself.

Source: (Uygen, 2004)

There are many levels of turbulence within an engine. Large-scale of turbulence occurs with eddies on the order of the size of the flow passage. For example valve opening or the height of the clearance volume. On the other extreme, the smallest scale turbulence is totally random and homogeneous, with no directionality and controlled by viscous dissipation. There are all levels of turbulence in between these extremes, with characteristics ranging from those of small scale turbulence to those of large scale of turbulence.

Local flame speed depends on the turbulence immediately in front of the flame. This turbulence is enhanced by the expansion of the cylinder gases during the combustion process. The shape of the combustion chamber is important in generating the maximum turbulence and increasing the desired rapid combustion. As speed is increase, turbulence increase and this increase the rate of evaporation, mixing and combustion. One result of this is that all engine speeds have about the same burn angle. One phase of this process that not changed due to the increasing turbulence is ignition delay. This is compensated for by advancing ignition spark timing which is initiate the spark earlier as the engine speed increased (Pulkrabek, 1997).

2.6 CHARACTERIZATION OF FLAMES

Combustion of the fuel-air mixture inside the engine cylinder is one of the processes that controls engine power, efficiency and emissions. In spark ignition engines, the fuel is normally mixed with air in the engine intake system. Following the compression of this fuel-air mixture is an electrical discharge initiates the combustion process which then creates a flame. A flame that develops from the “kernel” created by the spark discharge and propagates across the cylinder to the combustion chamber walls (Heywood, 1988).

Flames are usually classified according to the following overall characteristics. The first of these has to do with the composition of the reactants as they enter the reaction zone. The flame is designated as premixed if the fuel and oxidizer are essentially uniformly mixed together. The second means of classification relates to the basic character of the gas flow through the reaction zone. In laminar

flow, mixing and transport are done by molecular process. Laminar flows only occur at low Reynolds number. At high Reynolds number, turbulent flow occurs. In turbulent flows, mixing and transport are enhanced by the macroscopic relative motion of eddies or lumps of fluid which are the characteristic feature of a turbulent flow (Heywood, 1988).

2.7 FLAME STRUCTURE

The importance of the turbulence to the engine combustion process was recognized long ago through experiments where the intake event, and the turbulence it generates, was eliminated resulting with the rate of the flame propagation decreased substantially. Mixture burning rate is strongly influenced by engine speed. The duration of combustion in crank angle degrees only increases slowly with increasing engine speed. Additionally, at a given engine speed, increasing in-cylinder gas velocities increase the burning rate. Increasing engine speed and introducing swirl both increase the levels of turbulence in the engine cylinder at the time of combustion. With the increase in turbulence, this will increase the rate of development and propagation of turbulent premixed engine flame. Laminar flames in premixed fuel, air, residual gas mixtures are characterized by a laminar flame speed S_L and a laminar flame thickness δ_L . Turbulent flames are also characterized by the root mean square velocity fluctuation, the turbulence intensity u' , and the various length scale of the turbulent flow ahead of the flame (Heywood, 1988).

2.8 LAMINAR FLAME SPEED

Laminar burning velocity is an important intrinsic property of a combustible fuel, air and burned gas mixture. This burning velocity is defined as the velocity, relative to and normal to the flame front, with which unburned gas moves into the front and is transformed to products under laminar flow conditions. The flame front consists of two regions which is preheat zone and a reaction zone. In the preheat zone, the temperature of the unburned mixture is raised mainly by heat conduction from the reaction zone. The region between the temperature where exothermic chemical reaction begins and the hot boundary at the downstream equilibrium burned gas temperature is called the reaction zone. Laminar burning velocities at pressures and temperatures typical of unburned mixture in engines are usually measured in spherical closed vessels by propagating a laminar flame radially outward from the vessel center. The laminar burning velocity is given by (Heywood, 1988):

$$S_L = \frac{dm_b/dt}{A_f \rho_u} \quad (2.1)$$

Where the mass burning rate is determined from the rate of pressure rise in the vessel and A_f is the flame area. Data at higher pressures and temperatures have been fitted to a power law of the form (Heywood, 1988):

$$S_L = S_{L,o} \left(\frac{T_u}{T_o} \right)^\alpha \left(\frac{p}{p_o} \right)^\beta \quad (2.2)$$

Where $T_o = 298$ K and $p_o = 1$ atm are the reference temperature and pressure, and $S_{L,o}$, α and β are constant for a given fuel, equivalence ratio, and burned gas diluents fraction. For propane, isooctane and methanol, these constants can be represented by (Heywood, 1988):

$$\alpha = 2.18 - 0.8(\phi - 1) \quad (2.3)$$

$$\beta = -0.16 + 0.22(\phi - 1) \quad (2.4)$$

$$S_{L,o} = B_m + B_\phi(\phi - \phi_m)^2 \quad (2.5)$$

ϕ_m is the equivalence ratio at which $S_{L,o}$ is a maximum with value B_m .

Values of ϕ_m , B_m , and B_ϕ are given in Table 2.3.

Table 2.3: parameters for ϕ_m , B_m and B_ϕ

Fuel	ϕ_m	$B_m, \text{cm/s}$	$B_\phi, \text{cm/s}$
methanol	1.11	36.9	-140.5
Propane	1.08	34.2	-138.7
Isooctane	1.13	26.3	-84.7
Gasoline	1.21	30.5	-54.9

Source: (Heywood, 1988)

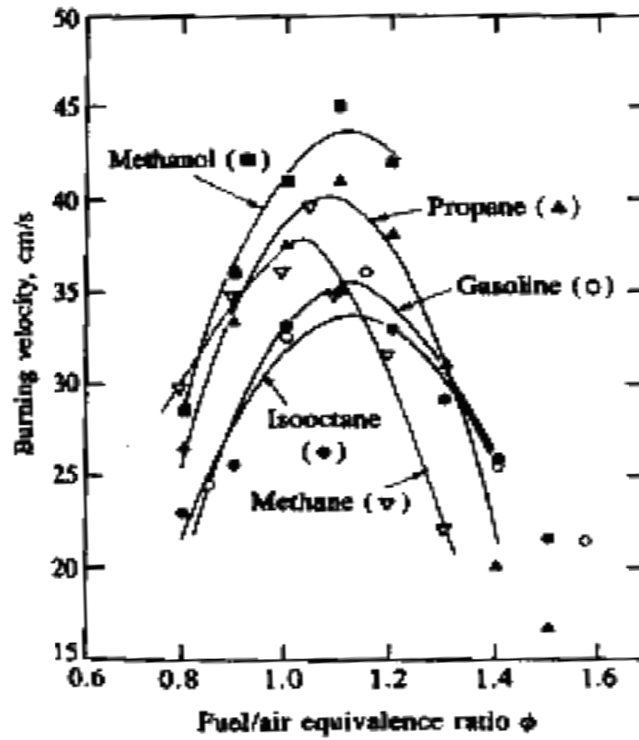


Figure 2.2: Laminar burning velocity for several fuels at 1 atm and 300 K

Source: (Heywood, 1988)

The presence of burned gas in the unburned cylinder charge due to residual gases and any recycled exhaust gases causes a substantial reduction in the laminar burning velocity. Any burned gas in the unburned mixture reduces the heating value per unit mass of mixture, thus reduces the adiabatic flame temperature. It acts as diluents. The proportional reduction in laminar burning velocity is essentially independent of the unburned mixture equivalence ratio, pressure and temperature over the range of interest in engines. The data are correlated by the relation (Heywood, 1988):

$$S_L(\tilde{x}_b) = S_L(\tilde{x}_b = 0)(1 - 2.06\tilde{x}_b^{0.77}) \quad (2.6)$$

\tilde{x}_b = the mole fraction of burned gas diluents.

2.9 TURBULENT FLAME SPEED

Due to their fundamental importance for premixed combustion theory, turbulent flame speed was a subject of a large number of investigations for many decades. Beginning with the classical work of Damköhler, turbulent flame speed by analogy with laminar flames has been assumed to be a basic characteristic of premixed turbulent combustion and has been the main focus of numerous experimental and theoretical studies (Lipatnikov, 2002). The first stage of the combustion is the ignition and flame development which is associated with burning of 5-10% of the cylinder mixture. The process is nearly laminar in nature at least at low to intermediate engine speed. There is only very small pressure and temperature rise during this period due to low mixture burned and consequently low energy released. Turbulent propagation flame is the next stage, where it is usually associated with 90-95% of mass fraction burned. The reaction sheet flame propagating outward in an approximately spherical manner. The thin reaction sheet flame is wrinkled by the turbulence motion at scale smaller than the flame radius. Comparable and larger scales of turbulence than the flame radius only distorted and convected the overall flame shape (Fadzil, 2008).

The effect of turbulence increases the flame propagation speed and the value is about 10 times faster than laminar flame front propagation. There are two mechanisms induced by turbulence, which is the wrinkling and stretching effect on the flame. By increasing the surface of thin reaction sheet within the turbulent flame zone, the burning rate increase by the wrinkling effect. While the stretching effects, which is produced by the wrinkling primarily, slowing down the burning rate by slowing the molecular diffusive process within the reaction sheet (Heywood, 1988). The mean reaction rate of the cylinder mixture is mostly governed by the three most important factors that is:

Table 2.4: important factors for mean reaction rate of cylinder mixture

Factors	Definition
Structure or geometry of the flame front	Highly influenced by the geometrical confinement of the flame.
Unburned mixture composition and state	Related with thermo-chemical properties
Turbulent flame speed	Govern the rate at which the flame front propagates across the combustion chamber

Source: (Fadzil, 2008)

In addition to the effects of turbulence, swirl and squish, the flame speed depends on the type of fuel and the air-fuel ratio. Lean mixtures have slower flame speeds. Rich mixtures have the fastest flame speeds, with the maximum for most fuels occurring at an equivalence ratio near 1.2. Exhaust residual and recycled exhaust gas slows the flame speed (Pulkrabek, 1997). As the flame propagates after the spark ignites, the cylinder mixtures that have been burned also increased. Turbulent flame speed is decrease as the flame front approaching the cylinder wall and this is where all the cylinder mixture has been completely burned.

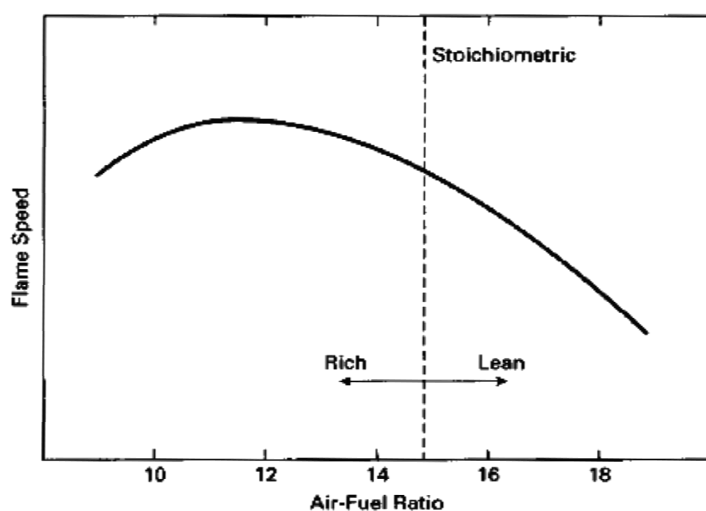


Figure 2.3: Flame speed in the combustion chamber of an SI engine as a function of the air-fuel ratio for gasoline-type fuels

Source: (Pulkrabek, 1997)

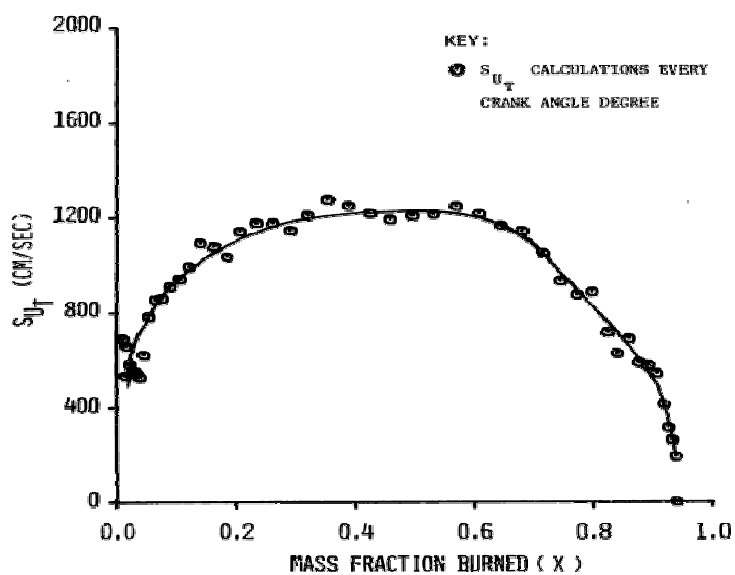


Figure 2.4: Turbulent flame speed against mass fraction burn

Source: (Larusso, 1976)

Turbulent flame flames have a propagation velocity that depends on the character of flow, as well as on mixture properties. Turbulent flame speed, S_t can be defined as the velocity at which unburned mixture enters the flame zone in a direction normal to the flame. Turbulent flame speed can be expressed as:

$$S_t = \frac{\dot{m}}{\bar{A}\rho_u} \quad (2.7)$$

Where the flame surface is represented as some time mean quantity. Instantaneous portions of the high temperature reaction zone may be largely fluctuating and usually been determined from measurement of reactant flow rates.

2.10 SUMMARY

This chapter has been discussed about the finding which relates to this study. The chapter has state about the combustion process in SI engine, turbulent flow, characterization of flame, also laminar and turbulent flame speed. From the findings, it is known that turbulent flame speed is one of the important parameter in SI engine combustion process. Thus a further step needs to be done aside from the findings.

CHAPTER 3

METHODOLOGY

3.1 INTRODUCTION

This chapter presents the main outline of the study which contains engine baseline specification, important parameters, numerical modeling approach, numerical analysis and the validation method.

3.2 BASELINE ENGINE SPECIFICATION

Table 3.1: Engine specification Mitsubishi Magma 4G15

Parameter	Size and Feature
Cylinder bore (mm)	75.5
Piston stroke (mm)	82
Compression ratio	9.2
Combustion chamber type	Pent-Roof type
Number valves per cylinder	3 valves per cylinder (two intake valves and one exhaust valve)
Intake valve open/closed	15° BTDC/63° ABDC
Exhaust valve open/closed	57° BBDC/13° ATDC

From Table 3.1, Mitsubishi magma 4G15 is taken as engine baseline to complete this project. The cylinder bore is 75.5 mm while piston stroke is 82.0 mm. The engine also has two intake valves and one exhaust valve with flat piston face. Since the engine combustion chamber type is pent-roof type, the development of top of combustion chamber is pent-roof type. From the table, the other important key of developing the computational domain is the compression ratio. The domain must obey the compression ratio which is 9.2 to simulating as it is.

3.3 ENGINE STRUCTURAL MODELING

After taking the dimension and also data from table 3.1, Solid work software was then used to create the model for this project. A 3D model engine design has been made based on the baseline engine specification. The dimension is based on the actual engine model used for Mitsubishi Magma 4G15. Engine model is design by making the intake and exhaust valve in overlap condition. Here is the result for the engine model:

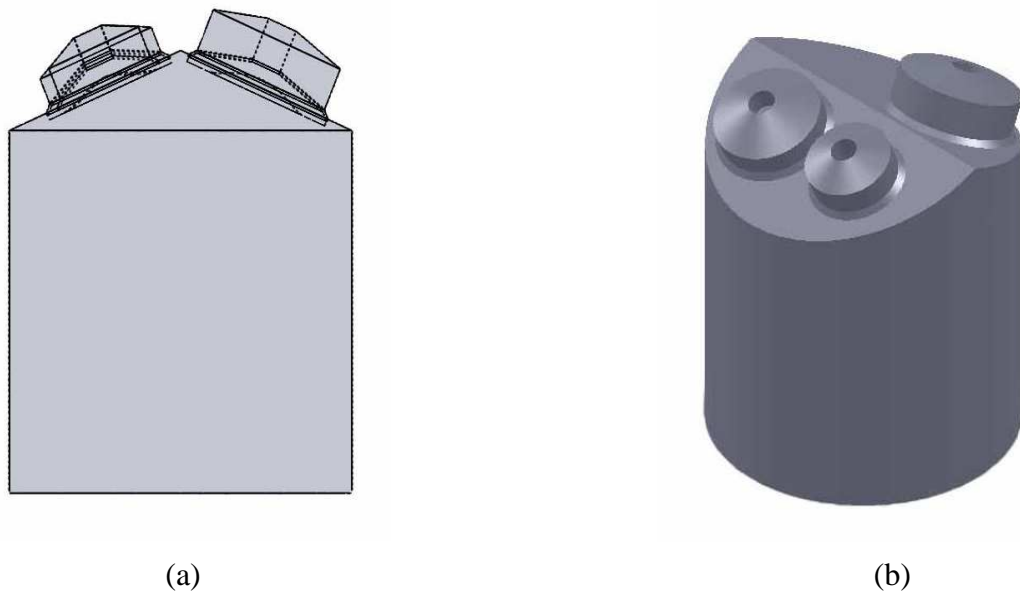


Figure 3.1: (a) Right view of the engine model where the intake and exhaust valve in overlap condition (hidden lines visible) and (b) Isometric view of the engine model (solid edge)

3.4 GRID GENERATION AND DOMAIN CREATION

The model that was created was then imported to ANSYS to start the grid generation or meshing process in order to simulate the actual engine motion. To define the deforming cylinder volume and valve face volume hexahedral meshed was used while for deforming combustion chamber tetrahedral meshed was used and is shown by figure 3.2. Moving boundary is selected for the piston face and the upper and lower faces of the valves. Stationary parts are defined for all manifolds and pent-roof walls.

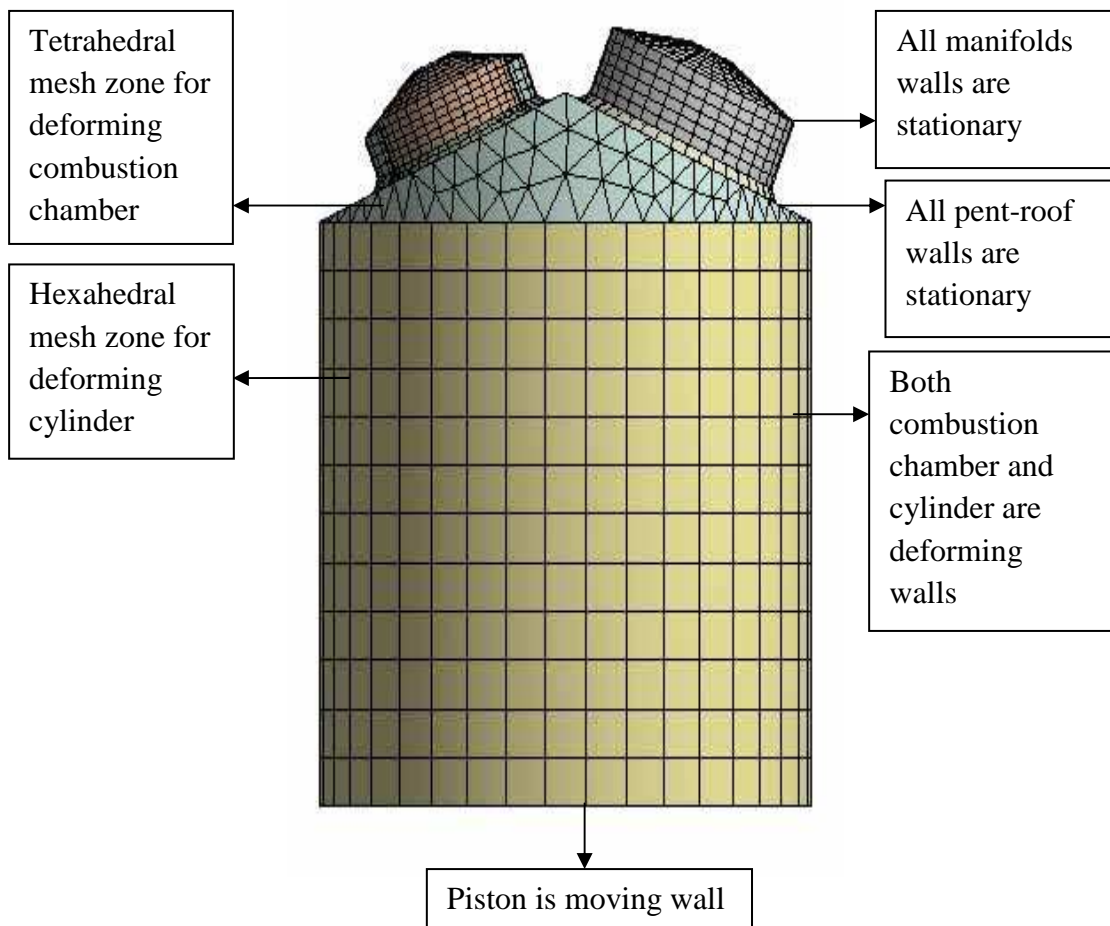


Figure 3.2: Engine meshing

3.5 GOVERNING EQUATION FOR COMPUTATIONAL FLUID DYNAMICS

CFD represent a vast area of numerical analysis in the field of fluid's flow phenomena. CFD is much more than just computer and numerical science. Since direct numerical solving of complex flows in real-like conditions requires an overwhelming amount of computational power success in solving such problem is very much dependent on the physical model applied. CFD methodology in FLUENT is using partial differential equations of flow variables to calculate and to simulate numerous kinds of analysis concerning the fluid flow. Among them is mass, momentum, energy, species concentration, quantities of turbulence and mixture fractions.

3.5.1 Mass Conservation Equation

The continuity equation or the mass conservation equation for any fluid flow is expressed as below (Fluent, 2004):

$$\frac{\partial}{\partial x} + \frac{\partial}{\partial x_j} (\rho u_j) = \dot{m} \quad (3.1)$$

where

- ρ : Fluid density
- u_j : The j th Cartesian component of instantaneous velocity
- \dot{m} : The rate of mass of the object generated in the system

This equation is valid for the incompressible and compressible flow. Moreover, the rate generated in the system, \dot{m} can be defined as the mass added to continues phase from the dispersed second phase such the vaporization of the liquid droplets and any other user-defined sources.

3.5.2 Momentum Conservation Equation

The conservation of momentum in i direction for an inertial reference frame can be explained as (Fluent, 2004):

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i \quad (3.2)$$

where

- ρ : Fluid density
- u_i & u_j : The i th and j th Cartesian components of the instantaneous velocity
- p : Static pressure
- τ_{ij} : Stressor tensor
- ρg_i : Gravitational body force
- F_i : External body force from interaction with dispersed phase in i direction

The stress tensor in Equation 3.2 is given as below:

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \left(\frac{\partial u_k}{\partial x_k} \right) \delta_{ij} \quad (3.3)$$

where

- μ : Fluid dynamic viscosity
- δ_{ij} : Kronecker delta

Note that the second term on the right hand side of Equation 3.2 describes the effect of volume dilation. By substituting Equation 3.3 into Equation 3.2, another equation is produced that is complete momentum conservation equation (Fluent, 2004):

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial p}{\partial x_j} \left\{ \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \left(\frac{\partial u_k}{\partial x_k} \right) \delta_{ij} \right\} \rho g_i + F_i \quad (3.4)$$

3.5.3 Energy Conservation Equation

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i} [u_i(\rho e + p)] = \frac{\partial}{\partial x_i} [K_{\text{eff}} \frac{\partial T}{\partial x_i} - \sum_j h_j J_j + u_j(\tau_{ij})_{\text{eff}}] + S_h \quad (3.5)$$

where

- K_{eff} : Effective conductivity
: $k + k_i$ (where k_i = turbulent thermal conductivity)
- J_j : Diffusion flux of species j
- S_h : Additional volumetric heat sources (example: heat of chemical reaction)
- h : Sensible enthalpy
- e : Specific total energy

The first three terms on the right-hand side of equation 3.5 represent the energy transfer due to conduction, species diffusion and viscous dissipation respectively. From equation 3.5 also, sensible enthalpy, h and specific total energy, e are defined as below:

$$e = h - \frac{p}{\rho} + \frac{ui^2}{2} \quad (3.6)$$

sensible enthalpy for ideal gas is defined as:

$$h = \sum_j m_j h_j \quad (3.7)$$

sensible enthalpy for incompressible flow is defined as:

$$h = \sum_j m_j h_j + \frac{p}{\rho} \quad (3.8)$$

where

- m_j : mass fraction of species j
- h_j : $\int_{T_{\text{ref}}}^T c_{p,j} dT$ with $T_{\text{ref}} = 298.15\text{K}$

3.6 PREMIXED COMBUSTION THEORY

Based on work by Zimont (Zimont, 2000), the turbulent premixed combustion model, involves the solution of a transport equation for the reaction progress variable. The closure of this equation is based on the definition of the turbulent flame speed.

3.6.1 Progress variable

As the flame front moves, combustion of unburnt reactants occurs, converting unburnt premixed reactants to burnt products. The premixed combustion model thus considers the reacting flow field to be divided into regions of burnt and unburnt species, separated by the flame sheet. The flame front propagation is modeled by solving a transport equation for the density-weighted mean reaction progress variable:

$$\frac{\partial \bar{\rho} \tilde{c}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{c}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\mu_T}{Sc_T} \frac{\partial \tilde{c}}{\partial x_j} \right) + \rho S_c \quad (3.9)$$

where

- \tilde{c} : Reaction progress variable
- Sc_T : Turbulent Schmidt number
- S_c : Reaction rate source term

The progress variable is defined as a normalized sum of the product species.

$$\tilde{c} = \frac{\sum_{k=1}^n Y_k}{\sum_{k=1}^n Y_{k,eq}} \quad (3.10)$$

where

- n : Total number of products
- Y_k : Mass fraction of product species k
- $Y_{k,eq}$: Equilibrium mass fraction of product species k